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This grant involved two different projects: The first one was focused on COIL flows and was performed during the first year The second one was focused on micro-ppt thrusters. Specifically, the objectives of this grant were as follows: (1) Numerical study of unsteadiness effects in the Chemical Oxygen Iodine (COIL) experiment conducted at Air Force Labs (year 1 only). (2) Develop spectral/hp element algorithms for the multi-species, compressible, viscous MHD equations for non-equalibrium plasma microflows in the continuous and transitional regimes (years 1-3). (3) Apply algorithms to modeling and optimization of micro-plasma thruster (micro-PPTs) (year 2-3).

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FINAL REPORT:
AFOSR number: F49620-00-1-0269
Mathematical and Computational Issues in Plasma Microthrusters

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Objectives

This grant involved two different projects: The first one was focused on COIL flows and was performed during the first year. The second one was focused on micro-ppt thrusters. Specifically, the objectives of this grant were as follows:

- Numerical study of unsteadiness effects in the Chemical Oxygen Iodine (COIL) experiment conducted at Air Force labs (year 1 only).
- Develop spectral/*hp* element algorithms for the multi-species, compressible, viscous MHD equations for non-equilibrium plasma microflows in the continuous and transitional regimes (years 1-3).
- Apply algorithms to modeling and optimization of micro-pulsed plasma thrusters (micro-PPTs) (years 2-3).

1 List of Accomplishments

1.1 High-Order Simulations of Coil Flows

NEKTAR is a high-order accurate code based on discontinuous Galerkin methods, developed under the sponsorship of AFOSR in previous grants. It uses hybrid discretizations, i.e. tetrahedra, hexahedra, prisms and pyramids or any combination of these. We have created a new mesh based on the surface geometry provided by Dr. T. Madden of Kirkland AFB. The important three-dimensional geometric details with the injection holes and the supersonic nozzle are resolved at very high accuracy.

Based on systematic direct numerical simulations, we have concluded that unsteadiness is suppressed in the supersonic conditions similar to the ones employed in the experiments. Our results are in good agreement with the results of Miller & Shang (AFB, Wright Patterson) who employed a steady-state finite volume code for this investigation. We have also obtained results for other flow conditions corresponding to subsonic and incompressible states. We found that in this case the flow is indeed unsteady. In addition, we have introduced "noise" in the supersonic COIL flow and carried out several simulations but in this case too the flow returned to steady state. The pressure distribution obtained from the direct numerical simulations is in agreement with available experimental results.

A typical result is shown in figure 1 for a supersonic and a subsonic state. The unsteadiness is clear only in the subsonic case, therefore the effect of compressibility is stabilizing.

1.2 Discontinuous Galerkin Methods for Plasma Micro-Thrusters

Micro-pulsed plasma thrusters (micro-PPTs) are characterized by complex physics and overlapping of electrodynamic, thermal, and hydrodynamic scales as well as transitional rarefaction effects. They achieve very high impulses at extremely low thrusts. Modeling micro-PPTs requires coupling of the teflon ablation process, of the electric circuit that triggers ignition, and of the magneto-hydrodynamic phenomena. The geometry is relatively simple but gradients and velocities are very large, i.e. in excess of 50 km/sec in a target size of about 100 microns.

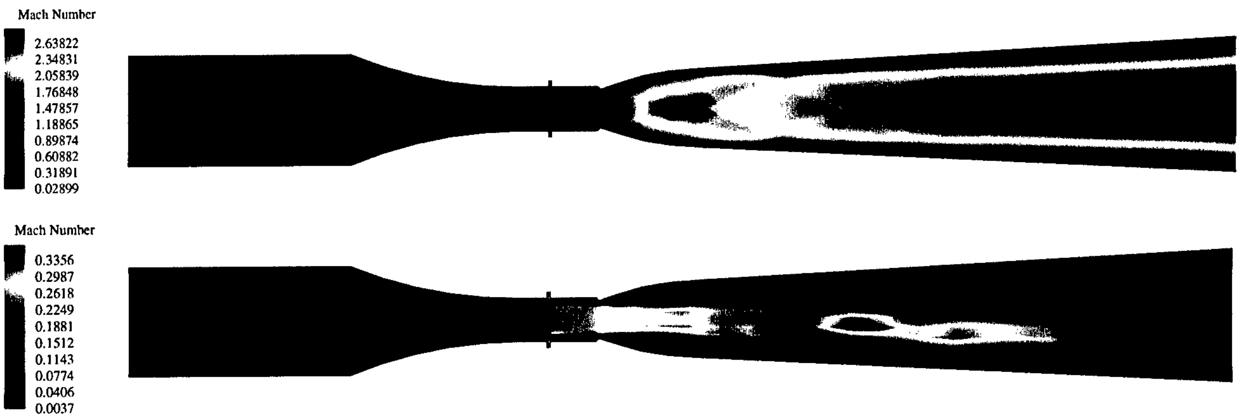

Figure 1: (Top) Supersonic flow in the COIL nozzle. (Bottom) Subsonic flow in the COIL nozzle. Plotted are contours of Mach number.

The main results that we obtained during in this grant address both *theory* and *applications.* We followed a hierarchical approach in dealing with the complexities of modeling non-equilibrium plasma in microscales: First, we modeled the plasma flow using one fluid and one temperature field. Subsequently, we employed one fluid but two temperature fields, i.e. separating the ion and electron energy equations. Finally, we adopted a two-fluid two-temperature approach. Specific algorithmic contributions include an entropy-based formulation, new slip boundary conditions, a stable penalty formulation, and an efficient algorithm for coupling thermal-electric and MHD domains. In the applications, we include several simulations to investigate the relative importance of the parameters that affect performance of the micro-PPT.

In the following, we provide a summary of the completed tasks.

- **Implementation and Verification of two-Temperature Model:** We have implemented the plasma equations in 1D, 2D and 3D using two energy equations (ions and electrons) appropriate for a single fluid, two-temperature plasma. The implementation for 1D is based on a standard ENO scheme while for the 2D and 3D NEKTAR versions is based on a discontinuous Galerkin method and spectral/*hp* element discretizations. Accuracy tests have shown the very fast convergence of the method for a magneto-hydrostatic problem as well as non-equilibrium effects in unsteady 2D and 3D plasma flows. Extensive work was done to efficiently parallelize the code using an MPI/C++ approach.

- **Implementation and Verification of two-Fluid Model:** The two fluid model assumes only local thermodynamic equilibrium and therefore can model micro-PPT flows more accurately. Here we have developed a 1D ENO code following the work of Dr. Uri Shumlak who has first pioneered this approach. The 1D algorithm allows for longitudinal and transverse magnetic fields and currents. In preliminary work we have performed simulations using the two-fluid model for the

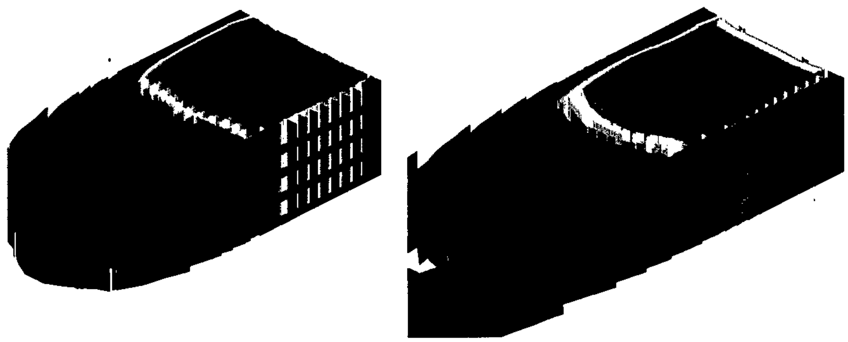

Figure 2: Three-dimensional micro-PPT simulations showing streamwise momentum 0.2 μ-sec (left) and 0.4 μ-sec (right) after start up.

Brio & Wu MHD shock. In this problem, the shock is completely determined by the Debye length and the gyro radius. The results show some subtle differences in comparison with the standard MHD approximation. More work is required to extend this more realistic two-fluid model to 2D and 3D using discontinuous Galerkin methods.

- This hierarchy of models and corresponding codes allows for very efficient resolution of design and optimization issues for new micro-PPTs.

• **Entropy-Based Formulation:** In micro-PPTs the size of density jump between inlet and outlet determines to a large degree the acceleration achieved and thus the micro-PPT effectiveness. However, dealing with the extremely small densities (almost vacuum) at the outlet is problematic. To this end, we have re-formulated the governing equations to include an entropy fix in regions with very low pressure. This is done dynamically in space and time and guarantees *positivity* of pressure/density at almost any conditions, including density jumps exceeding four orders of magnitude. We note that for MHD problems, the classical formulation is limited to about one order of magnitude in density jumps.

- This new hybrid formulation leads to a robust approach in handling extremely large density and pressure variations.

• **SESAME library:** One of the main issues in non-equilibrium plasma is the value of the transport coefficients and also the type of equation of state. Clearly, at temperatures exceeding 1 eV (about 12,000K), the ideal gas law is invalid while the semi-empirical equations for transport coefficients are also inaccurate. To this end, we have collaborated with researchers from Los Alamos and incorporated the SESAME library in the NEKTAR plasma codes, specifically the ones for teflon. This required interpolation and other software developments.

- Realistic transport coefficients and equations of state are key to correct predictions in simulating micro-PPTs.

• **Rarefaction Effects:** With target characteristic size of about 100 microns for the new generation of micro-PPTs, the corresponding Knudsen number is in the range 0.05 to 0.75, and thus significant rarefaction effects may be present. To this end, we have formulated and implemented new boundary conditions that account for velocity slip and temperature jumps. Unlike the classical Maxwell boundary condition, which is linear, our boundary condition is nonlinear and appropriate for both the slip flow as well as the transition regime. To implement efficiently this boundary condition, we have developed a penalty formulation and studied its stability.

- Velocity slip and temperature jump can be efficiently modeled using the new nonlinear boundary condition we have developed.

• **Mixed Domain Modeling:** The ablation of teflon determines the inlet velocity and the inlet temperature while the electric circuit determines the current waveform and corresponding magnetic field at the inlet. Therefore, these two thermal and electric domains are coupled to the MHD domain. To this end, we have developed a coupled formulation between the three *heterogeneous* domains and have studied its convergence for diverse conditions.

- Coupling ablation, electric circuit, and MHD is necessary for the accurate simulation of pulsed-plasma thrusters.

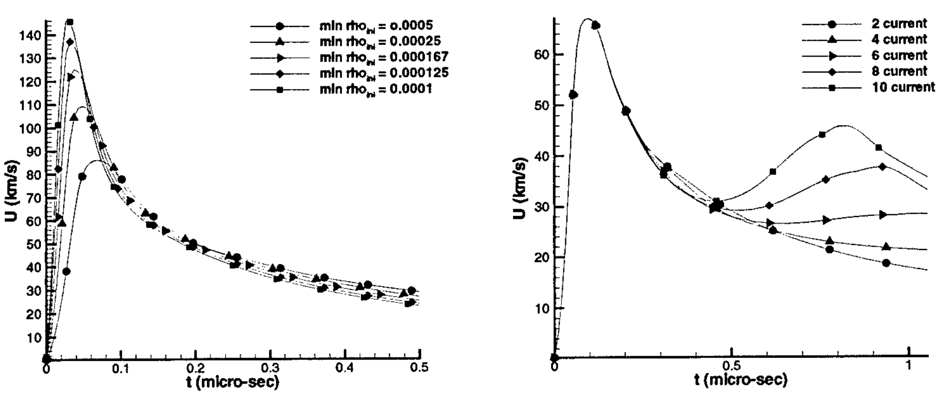

Figure 3: Effects of initial density jump (left) and of current waveforms (right) on the streamwise velocity.

• **Two- and Three-Dimensional Simulations of a Micro-PPT:** Using the NEKTAR-MHD code we have simulated several two- and three-dimensional designs of micro-PPTs. An example is shown in figure 2 which plots streamwise momentum contours at two time instants. Using the new codes optimization studies have been performed to investigate sensitivity of the effectiveness of the micro-PPT to various input parameters. In figure 3 we plot the results of variation of the initial jump in density and also of the current waveform. They show non-monotonic responses, which can be we are currently studying in order to propose an optimum micro-PPT design.

Personnel

- Faculty: G.E. Karniadakis, Professor of Applied Mathematics
- PhD Students: Guan Lin.

Publications

[1] I. Pivkin, R.M. Kirby and G.E. Karniadakis, "High-order discontinuous Galerkin methods: Simulation of COIL flows", Proc. Third AFOSR DNS/LES Conference, 2001.

[2] G. Lin and G.E. Karniadakis, "A High-order discontinuous Galerkin method for modeling micro pulsed plasma thrusters", Proc. International Electric Propulsion Conference, Pasadena, CA, 2001.

[3] G. Lin and G.E. Karniadakis, "High-order modeling of micro-pulsed plasma thrusters", AIAA 2002-2872, 32nd AIAA Fluid Dynamics Conference, June 2002, St. Louis.

[4] G. Lin and G.E. Karniadakis, "A discontinuous Galerkin method for non-equilibrium plasma flows", J. Comp. Phys., submitted, 2003.

Interactions/Transitions

The PI has been interacting closely with the other P.I. for this project. For example, for the COIL flows the PI has had useful interactions with Dr. Tim Madden of Kirkland AFB and Dr. Joe Shang of Wright Patterson. On the micro-ppt project the PI has had interactions with Prof. N. Gatsonis of WPI and with Prof. U. Shumlak of University of Washington.

- AFOSR Workshop on Microfluidics, USC, May 12-13, 2003.
- MIT, University of Illinois at Urbana-Champaign, University of Pennsylvania, WPI, and Northwestern University (invited).
- 32nd AIAA Summer Conference, June 2002 (invited).
- ECCOMAS 2001, Sweansa (**keynote**).
- International Conference on Modeling and Simulation of Microsystems, Hilton Head, (**keynote**).
- DARPA Workshop on Novel Applications of Microfluidics (invited).
- Nasa Langley/ICASE (invited).
- International Electric Propulsion Conference, IEPC2001 (Guan Lin).

Technology Transfer

The code **NEKTAR** is an *OpenSource* code that runs on all available platforms including Linux clusters of PCs. There is now documentation of the code both for users as well as developers.

The code has been distributed to several Universities and Laboratories. Some of them include:

- Kirkland AFB, Boeing, Inc., MIT, Caltech, UC Berkeley, Cornell University, Penn State University, University of Wisconsin, Imperial College, Oxford Computing Laboratory, University of Tokyo, University of Bologna, Norwegian University of Science & Technology, SUNY Buffalo, Texas A & M University, North Carolina University, Purdue University, Florida State University, Sandia National Labs, OAK Ridge National Labs, Nielsen, Inc. , the Mexican National Institute for Nuclear Research, Australian National University, Illinois Institute of Technology, Dresden University, University of Wales, University of Heidelberg, etc.

Acknowledgement/Disclaimer

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